Flow-Equation method for a superconductor with magnetic correlations

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Abstract

The flow equation method has been used to calculate the energy of single impurity in a superconductor for the Anderson model with $U \neq 0$.We showed that the energy of the impurity depends only of the Δ_R^2 (renormalized order parameter) which depends of the renormalized Hubbard repulsion U^R. For a strong Hubbard repulsion $U^R = U$ and $\Delta^R = \Delta^I$ the effect of the $s-d$ interactions are nonrelevant,a result which is expected for this model

Key Words: 2D superconductors,flow equations,magnetic correlations

1 Introduction

The flow equation method given by Wegner [1] has been successfully applied for the many-body problem by Kehrein and Mielke [2], for the Anderson Hamiltonian. In a previous paper the present authors [4] showed that this method can be used to calculate the energy of a superconductor containing magnetic impurities describe by the Anderson Hamiltonian. with $U = 0$. We studied (See ref.[4])the influence of the density of states on the single impurity energy for the case of a van-Hove density of states. In this case the energy is reduced by the superconducting state and corrections depends on Δ^2. In this paper we consider a superconductor with a constant density of states but for the impurity we take the Hubbard repulsion $U \neq 0$.

2 Model

We consider a superconductor containing magnetic impurities describe by the model Hamiltonian.:

$$H = H_{BCS} + H_A \tag{1}$$

where H_{BCS} is

$$H_{BCS} = \sum_{k,\sigma} \epsilon_k c^+_{k,\sigma} c_{k,\sigma} + \sum_k \Delta(c^+_{k,\uparrow} c^+_{-k,\downarrow} + c_{k,\uparrow} c_{-k,\downarrow}) \tag{2}$$

Δ being the order parameter and H_A the Anderson Hamiltonian. describing the impurity in a metal,as:

$$H_A = \sum_d \epsilon_d d^+_\sigma d_\sigma + \sum_{k,\sigma} V_{k,d}(c^+_{k,\sigma} d_\sigma + d^+_\sigma c_{k,\sigma}) + U d^+_\uparrow d^+_\downarrow d_\downarrow d_\uparrow \tag{3}$$

In equation (3) the first term is the energy of the impurities,the second term is the interaction between the itinerant-electron and impurity and the last term in the Hubbard repulsion between the d-electrons of the impurity. In order to make the problem analytically tractable we consider the case of a one impurity problem.

This problem has been treated using the flow-equation method by Crisan et.al. [4]for $U = 0$ and a van-Hove density of states. In the next section we consider the case $U \neq 0$ which is a more realistic case.

3 The Flow Equations

The flow equations method,which is in fact a renormalization procedure applied in the Hamiltonian formalism has been applied in the solid-state theory by the Wegner[1], Kehrein and Mielke [3] and has the main point the diagonalization of the Hamiltonian which describes the system by a continuous unitary transformation $\eta(l)$ which lead to a Hamiltonian. $H(l)$ with the parameters functions of the flow parameter l. This transformation satisfies:

$$\frac{dH(l)}{dl} = [\eta(l), H(l)] \tag{4}$$

where $\eta(l)$ can be calculated from:

$$\eta(l) = [H_0(l), H_{int}(l)] \tag{5}$$

In order to solve the differential equations using the Hamiltonian. (1) we introduce, following [2] the initial values:

$$\begin{aligned} \epsilon_k^I(l) &= \epsilon_k(l=0) \\ \epsilon_d^I(l) &= \epsilon_d(l=0) \\ V^I(l) &= V(l=0) \\ U^I(l) &= U(l=0) \end{aligned} \tag{6}$$

and the renormalized value for $l \to \infty$

$$\begin{aligned} \epsilon_k^R(l) &= \epsilon_k(\infty) \\ \epsilon_d^R(l) &= \epsilon_d(\infty) \\ V^R(l) &= V(\infty) \\ U^R(l) &= U(\infty) \end{aligned} \tag{7}$$

Using the Eq. (5) and the general method (see Ref.[1]) we calculate $\eta(l)$ as:

$$\eta(l) = \eta^{(0)}(l) + \eta^{(1)}(l) + \eta^{(2)}(l) + \eta^{(3)}(l) + \eta^{(4)}(l) \tag{8}$$

and obtain:

$$\begin{aligned} \eta^{(0)} &= \sum_{k,\sigma} \eta_k (c_{k,\sigma}^+ d_\sigma - d_\sigma^+ c_{k,\sigma}) \\ &+ \sum_{k,\sigma} \xi_k (d_{-\sigma}^+ c_{k,\sigma}^+ + c_{k,\sigma}^+ d_{-\sigma}) \end{aligned} \tag{9}$$

where:

$$\eta_k = (\epsilon_k - \epsilon_d)V_{k,d} \tag{10}$$

and:

$$\xi_{k,\sigma} = -\Delta V_{-k}\sigma \tag{11}$$

In Eq.(11) $\sigma = \uparrow, \downarrow$ correspond to $\sigma = \pm 1$ in the right side. The higher order contributions will be given as functions of expressions given by Eqs.(10) and (11) and by:

$$\Theta_{k,\sigma} = \eta_{-k}\Delta\sigma + \xi_{k,\sigma}\epsilon_d \tag{12}$$

as:

$$\eta^{(1)}_{k,\sigma} = (\epsilon_k V_k - \epsilon_d V_k - \Delta\Theta_{-k,\sigma}\sigma) \tag{13}$$

$$\eta^{(1)}_{k,k_1,\sigma} = \epsilon_k(\eta_{k,\sigma}V_{k_1} + \eta_{k_1,\sigma}V_k) - \Delta(\xi_{-k,\sigma}V_{k_1} - \xi_{k_1,\sigma}V_{-k})\sigma \tag{14}$$

$$\eta^{(2)}_{k,\sigma} = (-\Delta V_{-k}\sigma - \epsilon_k\Theta_{k,\sigma} - \epsilon_d\Theta_{k,\sigma}) \tag{15}$$

$$\eta^{(1)}_{k,k_1,\sigma} = [\Delta(\eta_{k_1\sigma}V_k + \eta_{k\sigma}V_{k_1})\sigma + \epsilon_k(\xi_{k1,\sigma}V_{-k} + \xi_{-k,\sigma}V_{k_1})] \tag{16}$$

$$\eta^{(3)}_{k,\sigma} = (\epsilon_k\eta_{k,\sigma}U - \epsilon_d\eta_{k,\sigma}U + \Delta U\xi_{-k,\sigma}\sigma) \tag{17}$$

$$\eta^{(4)}_{k,\sigma} = (\Delta\eta_{-k,\sigma}U\sigma - \epsilon_k\xi_k U - \epsilon_d\xi_k U) \tag{18}$$

If we take the spin orientation as $\sigma = 1$ (the non-magnetic states) the flow equations are:

$$\begin{aligned}
\frac{d\epsilon_d}{dl} &= -2\sum_k \eta^{(1)}_k V_k + 2\sum_k \eta^{(3)}_k V_k n_k \\
\frac{dV_k}{dl} &= \eta^{(1)}_k[\epsilon_k - \epsilon_d + \frac{U\Delta^2}{[U(1-n_k)+\epsilon_d+\epsilon_k][\epsilon_d - \epsilon_k + U] - \Delta^2}] \\
\frac{dU}{dl} &= -4\sum_k \eta^{(3)}_k V_k \\
\frac{d\Delta}{dl} &= \frac{1}{N(0)}\sum_k \eta^{(2)}_k V_{-k}
\end{aligned} \tag{19}$$

where n_k is the Fermi function.

4 Solutions of the flow equations

Using the spectral function

$$J(\epsilon,l)=\sum_k V_k^2\delta(\epsilon-\epsilon_k(l)) \tag{20}$$

and the factorization $\eta_k^{(1)}(l)=V_kf(\epsilon_k,l)$ the Eqs. (17) becomes as follows:

$$\frac{d\epsilon_d}{dl}-\int d\epsilon\frac{\partial J(\epsilon,l)}{\partial l}\frac{[\epsilon_d-\epsilon+U_1][\epsilon_d+\epsilon+U_2]-\Delta^2}{[\epsilon_d-\epsilon+U][\epsilon_d+\epsilon+U_2][\epsilon_d-\epsilon]-\Delta^2(\epsilon_d-\epsilon-U)} \tag{21}$$

where:

$$\begin{aligned} U_1 &= U(1+n(\epsilon)) \\ U_2 &= U(1-n(\epsilon)) \end{aligned} \tag{22}$$

The equation for U becomes:

$$\frac{dU}{dl}=2\int d\epsilon\frac{\partial J(\epsilon,l)}{\partial l}\frac{U[U_2+\epsilon_d+\epsilon]}{[\epsilon_d-\epsilon+U][\epsilon_d-\epsilon][U_2+\epsilon_d+\epsilon]-\Delta^2[\epsilon_d-\epsilon-U]} \tag{23}$$

These equations contain Δ^2 so we have to transform the equation for Δ as:

$$\frac{d\Delta^2}{dl}=\frac{1}{N(0)}\int d\epsilon\frac{\partial J(\epsilon,l)}{\partial l}\frac{2U\Delta^2n(\epsilon)}{[\epsilon_d-\epsilon+U][\epsilon_d-\epsilon][U_2+\epsilon_d+\epsilon]-\Delta^2[\epsilon_d-\epsilon-U]} \tag{24}$$

In the Eqs. (22),(23),(24)we have $\frac{\partial J(\epsilon,l)}{\partial l}$ which is obtained from Eqs. (18) as:

$$\frac{\partial J(\epsilon,l)}{\partial l}=2J(\epsilon,l)f(\epsilon,l)[\epsilon_d-\epsilon+\frac{U\Delta^2}{[\epsilon_d-\epsilon+U][U_2+\epsilon_d+\epsilon]-\Delta^2}] \tag{25}$$

and because we have this relation, a supplementary equation for $V_k(l)$ gives no more information about the system. The solutions of these equations will be obtained at $T=0$ $(n(\epsilon)=1-\Theta(\epsilon))$ and if we take a concrete form for the $J(\epsilon,l=0)$ as

$$J(\epsilon,l=0)=\frac{2V^2}{\pi D}=\frac{\Gamma}{\pi} \tag{26}$$

$\Gamma=\frac{2V^2}{\pi}$ where D is the bandwidth in the limit $U>>D>>\epsilon_d^R$ we obtained from Eqs.(19) using conditions (6),(7):

$$\begin{aligned} \epsilon_d^I &= \epsilon_d^R-\frac{\Gamma}{2\pi}\frac{\Delta_R^2}{\epsilon_d^{R2}}[1-\frac{\epsilon_d^R}{D}+arctanh\frac{D}{\epsilon_d^R}+ln\frac{D}{\epsilon_d^R}] \\ \Delta_I^2 &= \Delta_R^2(1+I_1) \\ U^I &= U^R+\frac{2\Gamma}{\pi}[ln\frac{\epsilon_d+D}{\epsilon_d-D}+ln\frac{\epsilon_d+U^R-D}{\epsilon_d^R+U^R+D}] \end{aligned} \tag{27}$$

where:

$$I_1 = -\frac{1}{2U^R(\epsilon_d^R+U^R)}[2ln\frac{\epsilon_d^R+U^R+D}{\epsilon_d^R+D}+ln\frac{\epsilon_d^{R2}}{\epsilon_d^{R2}-D^2}] + \frac{2(\epsilon_d^R+U^R)}{2U^R(2\epsilon_d^R+U^R)}arcth\frac{D}{\epsilon_d^R} \tag{28}$$

5 Conclusions

Using the flow equations method we showed that for a BCS superconductor with magnetic correlations describe by the Anderson Hamiltonian with $U \neq 0$ we calculated the energy of impurity ϵ_d the order parameter Δ and th e energy U. For a large D we get

$$\Delta_R = \Delta_I \qquad\qquad U^R = U^I \tag{29}$$

and th energy of the impurity presents a small variation as function of D.

References

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